

Quantum Coulomb Glass: Anderson localization in an interacting system

Thomas Vojta

Materials Science Institute, University of Oregon, Eugene, OR97403, USA

Frank Epperlein and Michael Schreiber

Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

(version August 25, compiled February 1, 2008)

The quantum Coulomb glass model describes disordered interacting electrons on the insulating side of a metal-insulator transition. By taking quantum fluctuations into account it can describe not only the localized limit but also the weakly localized regime. We discuss several possibilities to generalize the concept of Anderson localization to interacting electron systems such as the quantum Coulomb glass and define criteria for localization. The corresponding physical quantities are calculated by numerically exact diagonalization. The results indicate that single-particle excitations close to the Fermi energy become more strongly localized under the influence of interaction.

71.55.Jv, 72.15.Rn, 71.30.+h

I. INTRODUCTION

Disordered interacting electronic systems such as semiconductor impurity bands or granular metals have attracted a large amount of theoretical and experimental interest [1]. Even the presence of disorder or interaction alone leads to interesting phenomena, and the competition between the two gives rise to a very rich behavior. The single-electron states in non-interacting systems become localized in space for strong enough disorder. This phenomenon is called Anderson localization [2]; it is responsible for the metal-insulator transition in non-interacting systems. The generalization of this concept to interacting systems is not straightforward since many-particle physical properties cannot in general be derived from single-particle properties. Consequently, a definition of localization in many-particle systems will not be unique. In this paper we therefore consider several possibilities to generalize the concept of Anderson localization to interacting systems and discuss their relative merits. As an example we then apply the resulting localization criteria to the quantum Coulomb glass model of disordered insulators and calculate the corresponding physical quantities by numerically exact diagonalization.

The paper is organized as follows: In Sec. II we motivate and define the quantum Coulomb glass model. Sec. III is devoted to a discussion of Anderson localization in interacting systems and the presentation of our results. Sec. IV contains some discussions and conclusions.

II. FROM CLASSICAL TO QUANTUM COULOMB GLASS

Almost the entire current understanding of disordered insulators has been obtained from studying the insulating limit where the electrons are completely localized and can thus be described as classical point charges (we

will denote this regime as the classical insulating regime from now on). Although it is not a quantum mechanical system, the classical disordered insulator is a complicated many-body problem. Pollak predicted [3] an interaction-induced reduction of the single-particle DOS at the Fermi energy in disordered insulators. Later Efros and Shklovskii defined [4] the generic model of the classical insulating regime, the classical Coulomb glass model which consists of point charges in a random potential which interact via Coulomb interactions. The model is defined on a regular hypercubic lattice with $N = L^d$ (d is the spatial dimensionality) sites occupied by KN (spinless) electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of Ke . The Hamiltonian of the classical Coulomb glass reads

$$H_{cl} = \sum_i (\varphi_i - \mu) n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K) U_{ij}. \quad (1)$$

Here n_i is the occupation number of site i and μ is the chemical potential. The Coulomb interaction $U_{ij} = e^2/r_{ij}$ remains long-ranged since screening breaks down in the insulating phase. We set the interaction strength of nearest neighbor sites to 1 which fixes the energy scale. The random potential values φ_i are chosen independently from a box distribution of width $2W_0$ and zero mean. The physics of the classical Coulomb glass model has been investigated by several analytical and numerical methods and its properties are comparatively well understood by now [6] although the nature of the transport mechanism is still controversially discussed [7]. One of the remarkable features is the power-law gap in the zero-temperature single-particle density of states (DOS) which is called the Coulomb gap [4,5].

Since experiments deep in the insulating regime are difficult to carry out most results on disordered insulators have been obtained from samples not too far away

from the metal-insulator transition [8]. Here the (single-particle) localization length is still much larger than the typical distance between two sites and the description of the electrons in terms of classical point charges becomes questionable. In order to investigate the influence of finite overlap between the states on the properties of the insulating phase we have defined [9] the quantum Coulomb glass model, the minimal model of the "quantum insulating regime" which accounts for disorder, long-ranged interactions and the quantum nature of the electrons. It is obtained from the classical Coulomb glass by adding hopping matrix elements of strength t between nearest neighbors. The Hamiltonian of the quantum Coulomb glass reads

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + H_{\text{cl}}, \quad (2)$$

where c_i^\dagger and c_i are the electron creation and annihilation operators at site i , respectively, and the sum runs over all pairs of nearest neighbor sites. In the limit $t \rightarrow 0$ the model (2) reduces to the classical Coulomb glass, for vanishing Coulomb interaction but finite overlap it reduces to the usual Anderson model of localization.

III. LOCALIZATION IN AN INTERACTING SYSTEM

It has been known for a long time [10] that disorder leads to spatial localization of single-particle states in a non-interacting system. Since a system with localized states at the Fermi level is insulating, the transition between delocalized and localized states corresponds to a metal-insulator transition. There is, however, much experimental and theoretical evidence that a description of disordered electronic systems in terms of non-interacting particles is inadequate. For this reason one would like to apply the concept of localization to interacting systems. Unfortunately, a direct generalization of the non-interacting case is not possible since single-particle states are not defined in an interacting system while the many-particle states always correspond to extended charge distributions. The deeper reason for these difficulties is, of course, that in a non-interacting system the many-particle properties are completely determined by the single-particle properties whereas the same is not true for interacting systems. Therefore, in a many-particle system one can consider several types of "localization" (for single-particle or different many-particle excitations) which are all unrelated a priori. In this section we discuss some of these ideas and we also present results for the corresponding physical quantities of a two-dimensional quantum Coulomb glass.

From an experimental point of view the most natural quantity to consider is probably the conductance

since it is easily measurable and its behavior determines whether the system is metallic or insulating. However, since the conductance is given by a two-particle Greens function and involves complicated zero-temperature and zero-frequency limits it is difficult to calculate numerically [11].

In the following we concentrate on *single-particle localization* which is the most direct generalization of Anderson localization to many-body systems. Experimentally, single-particle localization should be reflected in the tunneling response of the system rather than in transport coefficients.

The simplest measure of Anderson localization for a single-particle state $|n\rangle$ is the participation number P , defined as the inverse second moment of the spatial probability distribution

$$P_n^{-1} = \sum_j |\langle n|j\rangle|^4 \quad (3)$$

where the sum runs over all sites j . In practice it is often averaged over all states with a certain energy ε

$$P^{-1}(\varepsilon) = \frac{1}{g(\varepsilon)} \frac{1}{N} \sum_n P_n^{-1} \delta(\varepsilon - \varepsilon_n). \quad (4)$$

A consistent generalization of this quantity to interacting systems should fulfill at least the following conditions: (i) it should be well defined for any many-particle state and (ii) it should reduce to (4) for non-interacting electrons. Moreover, the desired quantity should (iii) capture the physical idea of spatial localization and (iv) it should be easy to calculate.

It has been suggested to define localization in a many-particle system via the spatial distribution of the charge difference between the states of the same many-particle system with N and $N + 1$ particles, respectively. While this quantity fulfills the above conditions (i), (ii), and (iv) it turns out that it is *not* a useful measure of localization in a disordered interacting system. The reason is that adding an extra electron to a disordered interacting system will very often not only add some charge at a few sites but completely rearrange the distribution of all electrons due to the frustration introduced by the competition between disorder and interaction. Thus simply calculating the participation number of the extra charge leads to an overestimation of delocalization. This can already be seen at the example of the classical Coulomb glass where we know that the electrons are completely localized. Nevertheless the ground states of systems with N and $N + 1$ particles can be drastically different so that the charge difference between the two is distributed on more than one site, effectively giving a participation number larger than one. In general, the method will always fail, if adding an extra electron leads to a *decrease* of the charge at some particular site since then the charge

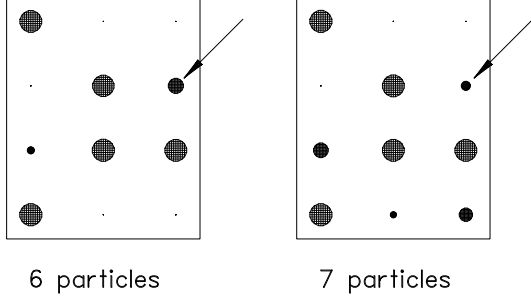


FIG. 1. Comparison of the ground states of quantum Coulomb glasses with 6 and 7 particles. The size of the circles is proportional to the charge density at the site. Note that adding an extra electron *reduces* the charge density at the site marked by an arrow.

density difference is not a proper probability distribution anymore (see Fig. 1).

There is, however, another quantity which fulfills conditions (i), (ii), and (iii) for a generalization of the inverse participation number. In particular, it nicely captures the physical idea of localization. This quantity is the probability R_p for an electron to return to its starting site in infinite time. The energy-dependent return probability can be expressed in terms of single-particle Greens functions

$$R_p(\varepsilon) = \frac{1}{N} \sum_j \lim_{\delta \rightarrow 0} \frac{\delta}{\pi} G_{jj}(\varepsilon + i\delta) G_{jj}(\varepsilon - i\delta). \quad (5)$$

For non-interacting electrons $P^{-1}(\varepsilon) = R_p(\varepsilon)$. We note, however, that calculating R_p requires the knowledge of all eigenstates of the Hamiltonian which makes this quantity numerically expensive. In Fig. 2 we show the numerically determined return probabilities of the quantum Coulomb glass and the Anderson model. The two systems behave very differently. For the Anderson model we obtain the well-known behavior of $P^{-1}(\varepsilon)$, viz. a minimum in the band center and higher values in the tails. In the quantum Coulomb glass the return probability has a maximum at the Fermi energy and decreases quickly with increasing distance from the Fermi energy. Thus we conclude that in the quantum Coulomb glass single-particle excitations away from the Fermi energy tend to delocalize while the excitations close to the Fermi energy which dominate the low-temperature physics tend to localize [14]. We have investigated the values of R_p close to the Fermi level for different values of the overlap t . In Fig. 3 we show the resulting dependence and the corresponding data for the Anderson model. The figure shows that for $t > 0.1$ the interactions lead to stronger localization in agreement with the results of our Hartree-Fock calculation [9]. For $t = 0.1$, quantum Coulomb glass and Anderson model show identical behavior within the numerical accuracy. Therefore, we cannot exclude that for

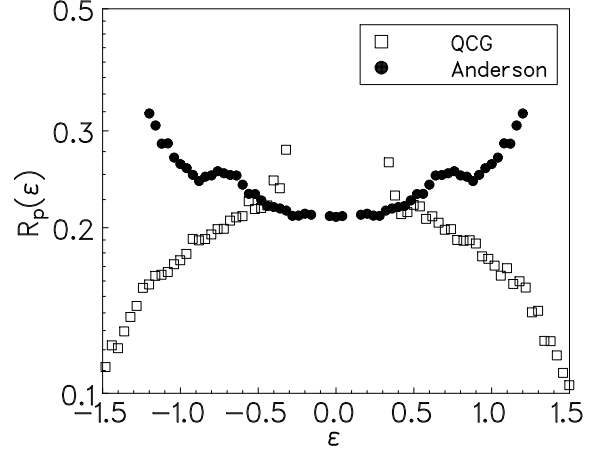


FIG. 2. Return probability for a quasiparticle in the quantum Coulomb glass and the Anderson model on a 3x4 lattice, $t = 0.3$, $W_0 = 1$, $K = 0.5$

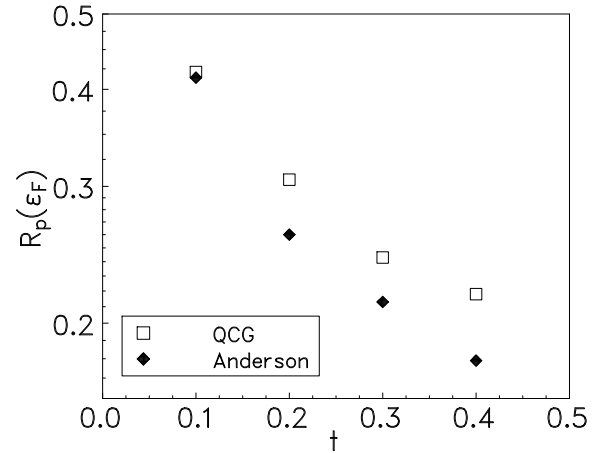


FIG. 3. Return probability for a quasiparticle at the Fermi energy as a function of t . Parameters are as in Fig. 2.

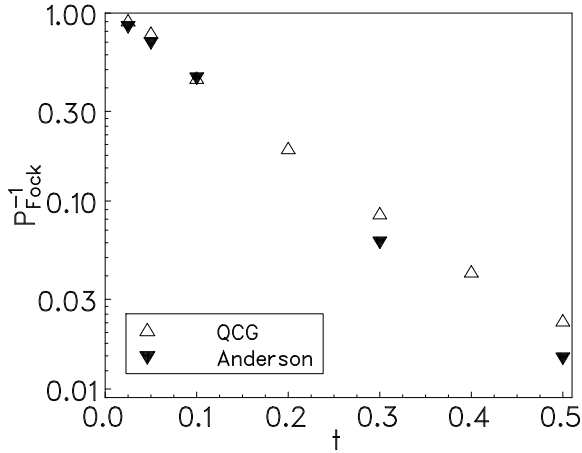


FIG. 4. Fock space participation numbers for the ground states of the quantum Coulomb glass and the Anderson model. Parameters are as in Fig. 2.

very small t , the behavior may turn around, i.e., the interactions may favor delocalization, see Ref. [13] and the discussion of Fock space localization below.

The return probability discussed above deals with the localization of a single quasiparticle. As already mentioned, in an interacting system many-particle properties cannot in general be derived from single-particle ones. Therefore, to get a complete understanding of the localization properties one has to investigate many-particle quantities, too [15]. One approach which is in some sense complementary to the study of the return probability is to analyze the localization properties of the many-particle states with respect to a Fock-space basis set $\{|\alpha\rangle\}$. Here the central quantity is the Fock-space participation number P_F of a many-body state $|\nu\rangle$ which is given by

$$P_F^{-1}(\nu) = \sum_{\alpha} |\langle \alpha | \nu \rangle|^4. \quad (6)$$

If we chose the Fock space basis to consist of Slater determinants of site basis functions, $|\alpha\rangle = c_i^\dagger \dots c_j^\dagger |0\rangle$ then $P_F = 1$ for completely localized electrons and $P_F > 1$ if the electrons can move. A measure like this has already been used to characterize the influence of long-range interactions on Anderson localization [13]. In Fig. 4 we present our results for the Fock-space participation numbers of the quantum Coulomb glass and the Anderson model. The data show the same tendency as the return probabilities at the Fermi level (Fig.3): For larger overlap t the interactions lead to stronger localization while for small t we cannot find a statistically significant difference between the quantum Coulomb glass and the Anderson model. Thus, a change in the behavior at very small t cannot be excluded. This would resolve the seeming disagreement with Ref. [13], where Fock space localization in a related model was investigated for very small

overlaps, and the authors found a delocalizing influence of the interactions. We note that, in principle, the concept of localization in Fock space can be applied to any problem in which the Hamiltonian can be decomposed into a reference part and a perturbation. Delocalization in Fock space then describes how the perturbation mixes the original eigenstates. In a recent letter [16] this concept has been applied to explain the transition in the width of excited states measured in tunneling conductance experiments in quantum dots [17].

Let us further mention that the localization transitions discussed above also lead to transitions of the statistics of the corresponding energy levels [9,13,18,19]. Analyzing the transitions of the level statistics is often numerically easier than dealing with the electron states itself.

IV. CONCLUSIONS

In this paper we have discussed the generalization of Anderson localization to interacting systems. We first have considered the localization of single-particle excitations which can be described in terms of the return probability R_p . Experimentally, this quantity should be reflected in the tunneling response of the system. We have also discussed the concept of Fock space localization for disordered interacting electron systems. As an example we have presented some numerical results for the quantum Coulomb glass model of disordered insulators. In this concluding section we will discuss some aspects that have not yet been covered. First, the quantum Coulomb glass is a model of spinless particles. In one-dimensional systems there is, however, some evidence that the electron spin plays an important role in determining the behavior of interacting disordered electrons [20]. Therefore, in order to describe real electrons, including the spin into the quantum Coulomb glass will be necessary in the future. Second, our numerical examples were for very small lattice sizes. In order to quantitatively analyze the behavior of disordered interacting electrons we have to extend the calculations to larger lattices. This can either be done by making approximations such as Hartree-Fock [9] or by developing better numerical algorithms. Third, one of the main tasks of the future will be to establish relations, if any, between the different types of localization and between the different quantities discussed here.

This work was supported in part by the DFG under grant nos. Schr231/13-1, Vo659/1-1 and SFB393 and by the NSF under grant no. DMR-95-10185.

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